Supporting Information

Ductility in Crystalline Boron Subphosphide ($B_{12}P_2$) for Large Strain Indentation

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Table S1. The predicted bulk modulus (unit: GPa), shear modulus (unit: GPa), hardness (unit: GPa), ideal shear stress (unit: GPa), and critical stress under biaxial shear (unit: GPa) for both crystalline and nanotwinned $B_{12}P_2$.

Structure	Crystalline $B_{12}P_2$	Nanotwinned $B_{12}P_2$
Bulk modulus (Voigt)	199.8	199.1
Bulk modulus (Reuss)	198.4	198.3
Bulk modulus (V-R-H)	199.1	198.7
Shear modulus (Voigt)	191.2	190.2
Shear modulus (Reuss)	190.5	190.0
Shear modulus (V-R-H)	190.9	190.1
Theoretical Vickers hardness	38.1	37.9
Ideal shear stress	44.2	42.6
Critical shear stress under biaxial shear deformation	27.7	26.9

Table S2. The predicted elastic constant (unit: GPa) for crystalline $B_{12}P_2$

C_{ij}	XX	YY	ZZ	XY	YZ	ZX
XX	439.60	66.70	74.07	-11.48	-13.77	-8.8
YY	66.70	455.82	81.96	-10.31	0.66	-10.05
ZZ	74.07	81.96	457.70	-10.59	-4.16	-5.99
XY	-11.48	-10.31	-10.59	189.14	-3.61	-9.29
YZ	-13.77	0.66	-4.16	-3.61	195.76	-2.20
ZX	-8.81	-10.05	-5.99	-9.29	-2.20	194.12

Table S3. The predicted elastic constant (unit: GPa) for nanotwinned $B_{12}P_2$

C_{ij}	XX	YY	ZZ	XY	YZ	ZX
XX	436.33	74.03	67.20	0.00	0.00	10.99
YY	74.03	448.60	84.01	0.00	0.00	10.57
ZZ	67.20	84.01	456.60	0.00	0.00	10.47
XY	0.00	0.00	0.00	194.57	0.79	0.00
YZ	0.00	0.00	0.00	0.79	195.31	0.00
ZX	10.99	10.57	10.47	0.00	0.00	189.20